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Dynamic Microscopic Theory of Fusion Using DC-TDHF

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Abstract. The density-constrained time-dependent Hartree-Fock (DC-TDHF) theory is a fully microscopic approach for calculating heavy-ion interaction potentials and fusion cross sections below and above the fusion barrier. We discuss recent applications of DC-TDHF method to fusion of light and heavy systems.

Keywords: TDHF, density constraint, fusion barrier

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INTRODUCTION

The investigation of internuclear potentials for heavy-ion collisions is of fundamental importance for the study of fusion reactions as well as for the formation of superheavy elements and nuclei far from stability. Recently, we have developed a new method to extract ion-ion interaction potentials directly from the time-dependent Hartree-Fock (TDHF) time-evolution of the nuclear system [1]. In the density-constrained TDHF (DC-TDHF) approach the TDHF time-evolution takes place with no restrictions. At certain times during the evolution the instantaneous density is used to perform a static Hartree-Fock minimization while holding the neutron and proton densities constrained to be the corresponding instantaneous TDHF densities. In essence, this provides us with the TDHF dynamical path in relation to the multi-dimensional static energy surface of the combined nuclear system. Since TDHF directly provides us with the most probable fusion path in the mean-field limit there is no need calculate the entire PES to determine the fusion path as in the case of computation of fission barriers. In short, we have a self-organizing system which selects its evolutionary path by itself following the microscopic dynamics. Some of the effects naturally included in the DC-TDHF calculations are: neck formation, mass exchange, internal excitations, deformation effects to all order, as well as the effect of nuclear alignment for deformed systems. The DC-TDHF theory provides

a comprehensive approach to calculating fusion barriers in the mean-field limit. The theory has been applied to calculate fusion cross-sections for large number of systems [1, 2]. In this proceeding we will outline the DC-TDHF method and give examples of its application to the calculation of fusion cross-sections for various systems.

THEORY

In the DC-TDHF approach, the time-evolution takes place with no restrictions. At certain times t or, equivalently, at certain internuclear distances $R(t)$ the instantaneous TDHF density

$$\rho_{\text{TDHF}}(r, t) = \langle \Phi(t) | \rho | \Phi(t) \rangle \quad (1)$$

is used to perform a static Hartree-Fock energy minimization

$$\delta \langle \Phi_\rho | H - \int d^3r \lambda(r) \rho(r) | \Phi_\rho \rangle = 0 \quad (2)$$

while constraining the proton and neutron densities to be equal to the instantaneous TDHF densities

$$\langle \Phi_\rho | \rho | \Phi_\rho \rangle = \rho_{\text{TDHF}}(r, t) . \quad (3)$$

These equations determine the state vector Φ_ρ . This means we allow the single-particle wave functions to rearrange themselves in such a way that the total energy is minimized, subject to the TDHF density constraint. In a typical DC-TDHF run, we utilize a few thousand time steps, and the density constraint is applied every 20 time steps. We refer to the minimized energy as the “density constrained energy” $E_{\text{DC}}(R)$

$$E_{\text{DC}}(R) = \langle \Phi_\rho | H | \Phi_\rho \rangle . \quad (4)$$

The ion-ion interaction potential $V(R)$ is essentially the same as $E_{\text{DC}}(R)$, except that it is renormalized by subtracting the constant binding energies E_{A_1} and E_{A_2} of the two individual nuclei

$$V(R) = E_{\text{DC}}(R) - E_{A_1} - E_{A_2} . \quad (5)$$

The interaction potentials calculated with the DC-TDHF method incorporate all of the dynamical entrance channel effects present in the mean-field dynamics, such as neck formation, particle exchange, internal excitations, and deformation effects. While the outer part of the potential barrier is largely determined by the entrance channel properties, the inner part of the potential barrier is strongly sensitive to dynamical effects such as particle transfer and neck formation.

Using TDHF dynamics, it is also possible to compute the corresponding coordinate dependent mass parameter $M(R)$ using energy conservation at zero impact parameter. As expected, at large distance R the mass $M(R)$ is equal to the reduced mass μ of the system. In general, we observe that the coordinate-dependent mass changes only the interior region of the potential barriers, and this change is most pronounced at low $E_{\text{c.m.}}$ energies. Fusion cross-sections are calculated by numerically integrating the Schrödinger equation using the well-established *Incoming Wave Boundary Condition* (IWBC) method [3].

RESULTS

In this Section we give some recent examples of DC-TDHF calculations of heavy-ion potentials and cross-sections. Fusion of very neutron rich nuclei may be important to determine the composition and heating of the crust of accreting neutron stars [4]. In Fig. 1a we show the DC-TDHF potential barriers for the C+O system. The higher barrier corresponds to the $^{12}\text{C} + ^{16}\text{O}$ system and has a peak energy of 7.77 MeV. The barrier for the $^{12}\text{C} + ^{24}\text{O}$ system occurs at a slightly larger R value with a barrier peak of 6.64 MeV. Figure 1b shows the corresponding cross sections for the two reactions. Also shown are the experimental data from Ref. [5]. The DC-TDHF potential reproduces the experimental cross-sections quite well for the $^{12}\text{C} + ^{16}\text{O}$ system, and the cross section for the neutron rich $^{12}\text{C} + ^{24}\text{O}$ is predicted to be larger than that for $^{12}\text{C} + ^{16}\text{O}$.

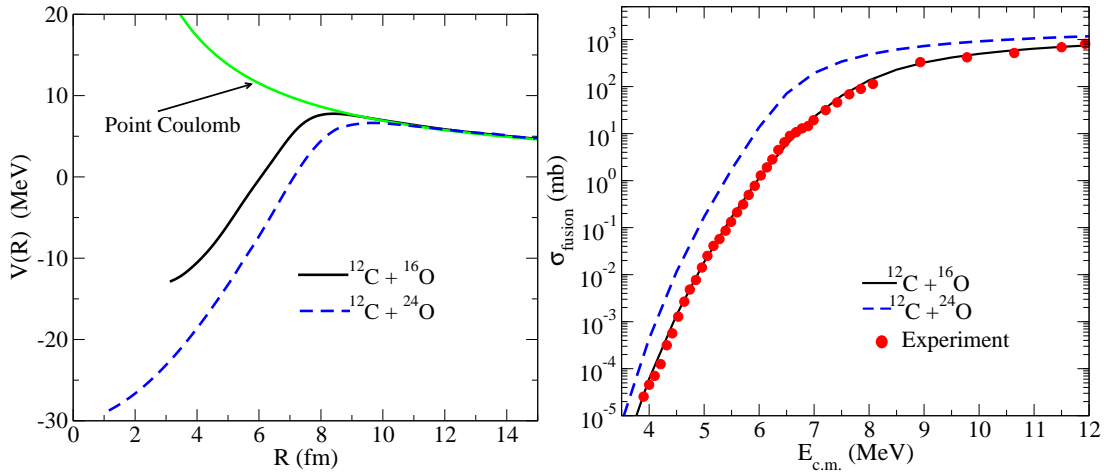


FIGURE 1. (a) Ion-Ion potential for various isotopes of the C+O system. (b) Corresponding cross-sections.

Figures 2a and Fig. 2b show the corresponding potentials and cross-sections for the Ca+Ca system [6], which was the subject of recent experimental studies [7]. The observed trend for sub-barrier energies is typical for DC-TDHF calculations when the underlying microscopic interaction gives a good representation of the participating nuclei. Namely, the potential barrier corresponding to the lowest collision energy gives the best fit to the sub-barrier cross-sections since this is the one that allows for more rearrangements to take place and grows the inner part of the barrier. Considering the fact that historically the low-energy sub-barrier cross-sections of the $^{40}\text{Ca} + ^{48}\text{Ca}$ system have been the ones not reproduced well by the standard models, the DC-TDHF results are quite satisfactory, indicating that the dynamical evolution of the nuclear density in TDHF gives a good overall description of the collision process. The shift of the cross-section curve with increasing collision energy is typical. In principle one could perform a DC-TDHF calculation at each energy above the barrier and use that cross-section for that energy. However, this would make the computations extremely time consuming and may not provide much more insight. The trend at higher energies for the $^{40}\text{Ca} + ^{48}\text{Ca}$ system is atypical. The calculated cross-sections are larger than the experimental ones by about a factor of two. Such lowering of fusion cross-sections with increasing collision energy is commonly seen in lighter systems where various inelastic channels, clustering,

and molecular formations are believed to be the contributing factors.

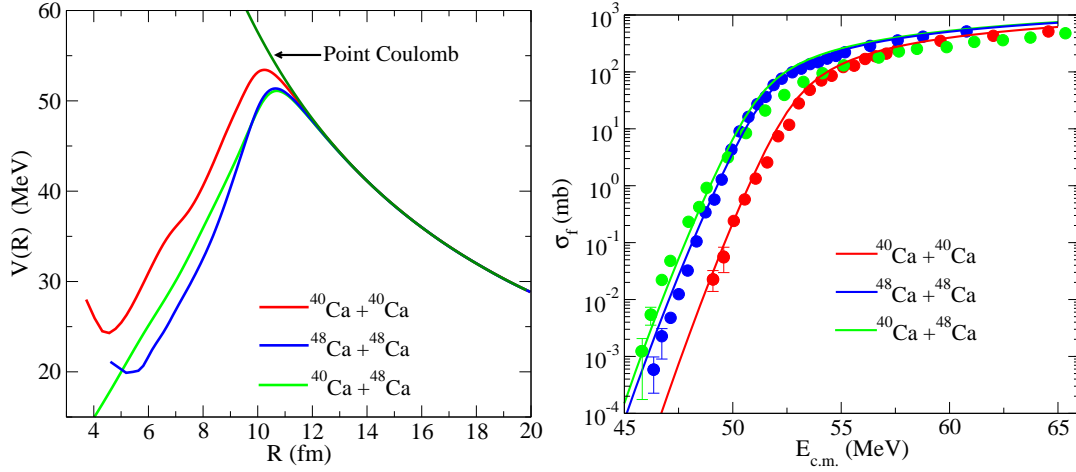


FIGURE 2. (a) Ion-Ion potential for various isotopes of the Ca+Ca system. (b) Corresponding cross-sections.

CONCLUSIONS

The fully microscopic TDHF theory has shown itself to be rich in nuclear phenomena and continues to stimulate our understanding of nuclear dynamics. The time-dependent mean-field studies seem to show that the dynamic evolution builds up correlations that are not present in the static theory. While modern Skyrme forces provide a much better description of static nuclear properties in comparison to the earlier parametrizations there is a need to obtain even better parametrizations that incorporate deformation and reaction data into the fit process.

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